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Poly[[μ -aqua-tetraaquabis(μ -2-hydroxy-4-oxocyclobut-1-ene-1,3-diolato)-strontium] hemihydrate]

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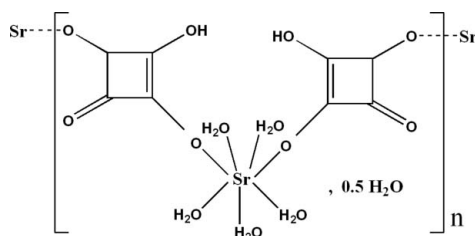
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Key indicators: single-crystal X-ray study; $T = 150$ K; mean $\sigma(\text{C}—\text{C}) = 0.004$ Å; R factor = 0.028; wR factor = 0.068; data-to-parameter ratio = 12.6.

In the title coordination polymer, $[\text{Sr}(\text{C}_4\text{HO}_4)_2(\text{H}_2\text{O})_5] \cdot 0.5\text{H}_2\text{O}$, the Sr^{2+} ion is coordinated by three monodentate hydrogensquarate (hsq) anions and six aqua ligands in a distorted SrO_9 monocapped square-antiprismatic geometry. The hsq anions and water molecules bridge the metal ions into infinite sheets lying parallel to (100). The O atom of the uncoordinated water molecule lies on a crystallographic twofold axis. The packing is stabilized by numerous $\text{O}—\text{H} \cdots \text{O}$ hydrogen bonds.

Related literature

For the isostructural mixed-metal Ba/Sr analogue of the title compound and background references, see: Trifa *et al.* (2011).



Experimental

Crystal data

$[\text{Sr}(\text{C}_4\text{HO}_4)_2(\text{H}_2\text{O})_5] \cdot 0.5\text{H}_2\text{O}$

$M_r = 412.81$

Monoclinic, $C2/c$

$a = 24.885$ (3) Å

$b = 8.8026$ (9) Å

$c = 13.8918$ (17) Å

$\beta = 119.609$ (4)°

$V = 2645.7$ (5) Å³

$Z = 8$

Mo $K\alpha$ radiation

$\mu = 4.15$ mm^{−1}

$T = 150$ K

$0.57 \times 0.27 \times 0.10$ mm

Data collection

Bruker APEXII diffractometer

Absorption correction: multi-scan

SADABS (Bruker, 2006)

$T_{\min} = 0.365$, $T_{\max} = 0.660$

9165 measured reflections

3006 independent reflections

2243 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.037$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$

$wR(F^2) = 0.068$

$S = 1.03$

3006 reflections

239 parameters

2 restraints

H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{\text{max}} = 0.42$ e Å^{−3}

$\Delta\rho_{\text{min}} = -0.51$ e Å^{−3}

Table 1

Selected bond lengths (Å).

Sr1—O1	2.691 (2)	Sr1—O6	2.6179 (18)
Sr1—O2	2.642 (2)	Sr1—O12	2.6646 (16)
Sr1—O3	2.690 (2)	Sr1—O14 ⁱ	2.5906 (16)
Sr1—O4	2.641 (3)	Sr1—O3 ⁱⁱ	2.7154 (19)
Sr1—O5	2.572 (2)		

Symmetry codes: (i) $x, y + 1, z$; (ii) $-x + 2, -y + 2, -z + 1$.

Table 2

Hydrogen-bond geometry (Å, °).

$D—H \cdots A$	$D—H$	$H \cdots A$	$D \cdots A$	$D—H \cdots A$
O1—H1A ⁱⁱⁱ ···O9 ⁱⁱⁱ	0.76 (4)	2.27 (4)	2.983 (3)	158 (4)
O1—H1B ^{iv} ···O7 ^{iv}	0.79 (4)	1.99 (4)	2.715 (2)	153 (4)
O1W—H1W ^v ···O13 ⁱⁱ	0.76 (2)	2.39 (2)	2.801 (2)	115 (2)
O1W—H1W ^v ···O8 ^v	0.76 (2)	2.51 (3)	3.118 (2)	138 (3)
O2—H2A ^{vi} ···O14 ^{vi}	0.92 (4)	1.91 (4)	2.794 (3)	161 (4)
O2—H2B ^{vii} ···O1W ^{vii}	0.70 (4)	2.52 (4)	3.165 (3)	154 (4)
O3—H3A ⁱⁱ ···O13 ⁱⁱ	0.93 (4)	1.79 (4)	2.712 (3)	174 (3)
O3—H3B ^{viii} ···O4 ^{viii}	0.76 (4)	2.59 (4)	3.172 (3)	136 (3)
O4—H4A ^{ix} ···O7 ^{ix}	0.78 (4)	2.01 (4)	2.785 (3)	177 (4)
O4—H4B ^x ···O1W	0.87 (4)	2.03 (4)	2.871 (3)	163 (3)
O5—H5A ^x ···O1 ^x	0.72 (4)	2.09 (4)	2.787 (3)	166 (4)
O5—H5B ^{xi} ···O8 ^{xi}	0.90 (4)	1.82 (4)	2.716 (3)	175 (4)
O9—H9 ^x ···O12	0.82	1.74	2.548 (3)	169
O11—H11 ^x ···O6 ^{vii}	0.82	1.77	2.580 (2)	172

Symmetry codes: (ii) $-x + 2, -y + 2, -z + 1$; (iii) $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$; (iv) $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$; (v) $x + \frac{1}{2}, -y + \frac{5}{2}, z + \frac{1}{2}$; (vi) $-x + 2, -y + 1, -z + 1$; (vii) $x, y - 1, z$; (viii) $-x + 2, y, -z + \frac{1}{2}$; (ix) $-x + \frac{3}{2}, -y + \frac{5}{2}, -z$; (x) $x, -y + 2, z - \frac{1}{2}$; (xi) $-x + \frac{3}{2}, -y + \frac{3}{2}, -z$.

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg & Berndt, 2001); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5939).

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